

10/566,252

STN-Structure Search  
9/29/06

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Inventor

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:120883 CAPLUS  
 DOCUMENT NUMBER: 142:219153  
 TITLE: Preparation of (piperidylalkyl)benzylamine derivatives  
 as tachykinin receptors antagonists  
 INVENTOR(S): Nagasawa, Masaaki; Kawase, Nobuo; Tanaka, Nobuyuki;  
 Nakamura, Hideki; Tsuzuike, Naoki; Murata, Masakazu  
 PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 248 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012248	A1	20050210	WO 2004-JP11065	20040802
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004261534	A1	20050210	AU 2004-261534	20040802
CA 2534460	AA	20050210	CA 2004-2534460	20040802
EP 1650189	A1	20060426	EP 2004-748198	20040802
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
CN 1829689	A	20060906	CN 2004-80021890	20040802
US 2006194841	A1	20060831	US 2006-566252	20060130
PRIORITY APPLN. INFO.:			JP 2003-205114	A 20030731
			WO 2004-JP11065	W 20040802
OTHER SOURCE(S):	MARPAT 142:219153			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. I [wherein X1 = NMe, NH, or O; X2 = a single bond, NH, CONH, O, S, etc.; X3 and X4 = independently H or halo; R1 = H, alkyl, (un)substituted Ph, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = alkanoylamino, aminoalkanoyl, aminoalkanoylamino, etc.; R4 = H or forming a ring with R3; R5 = H or alkyl; m = 1 or 2; n = 0 or 1] or salts thereof are prepared as tachykinin receptors (NK) antagonists. For example, the compound II was prepared in a multi-step synthesis. II showed antagonistic activity with IC50 of 0.9 nM against human NK1. I are useful for the treatment of irritable bowel syndrome, pain, anxiety, obstructive bronchial diseases, headache, and vomiting (no data).

IT 841255-89-8P 841255-92-3P 841255-93-4P  
 841255-94-5P 841255-95-6P 841255-96-7P  
 841255-97-8P 841256-39-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

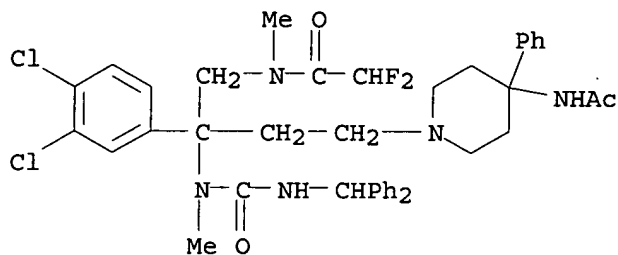
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(Uses)

(drug candidate; preparation of (piperidylalkyl)benzylamine derivs. as tachykinin receptors antagonists)

RN 841255-89-8 CAPLUS

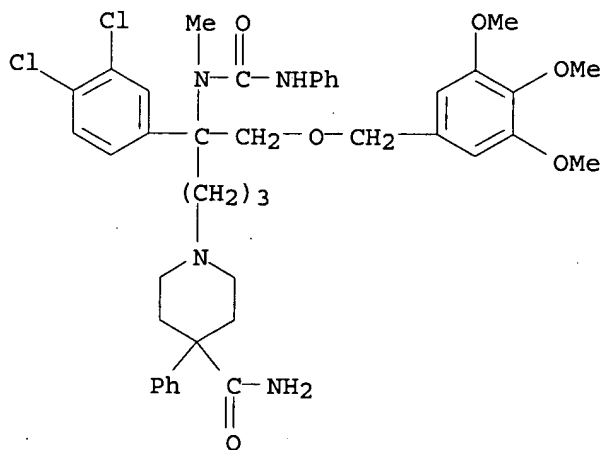
CN Acetamide, N-[4-[4-(acetylamino)-4-phenyl-1-piperidinyl]-2-(3,4-dichlorophenyl)-2-[[[(diphenylmethyl)amino]carbonyl]methylamino]butyl]-2,2-difluoro-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 841255-92-3 CAPLUS

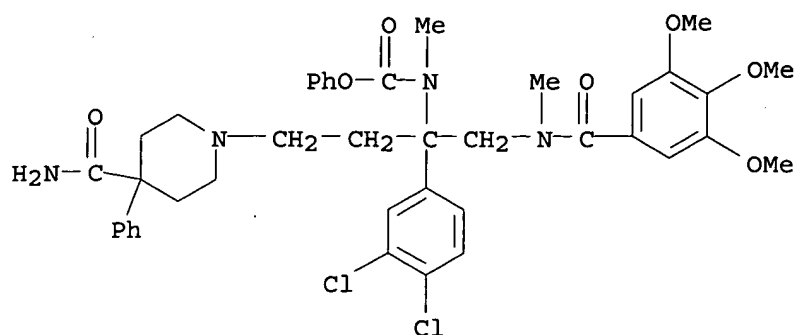
CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-[methyl[(phenylamino)carbonyl]amino]-5-[(3,4,5-trimethoxyphenyl)methoxy]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 841255-93-4 CAPLUS

CN Carbamic acid, [3-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-dichlorophenyl)-1-[[methyl(3,4,5-trimethoxybenzoyl)amino]methyl]propyl]methyl-, phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

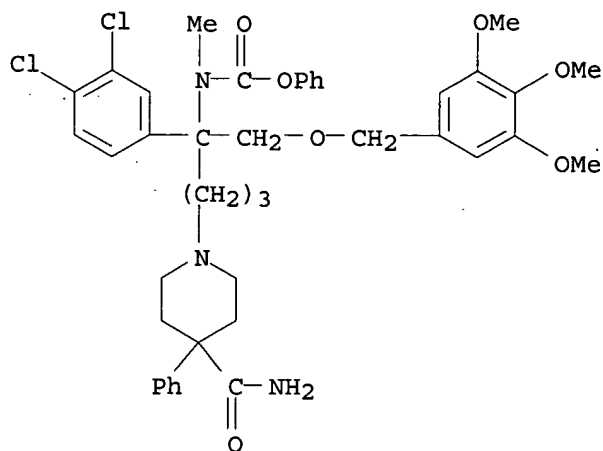
10/566,252



● HCl

RN 841255-94-5 CAPLUS

CN Carbamic acid, [4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-dichlorophenyl)-1-[(3,4,5-trimethoxyphenyl)methoxy]methyl]butyl]methyl-, phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

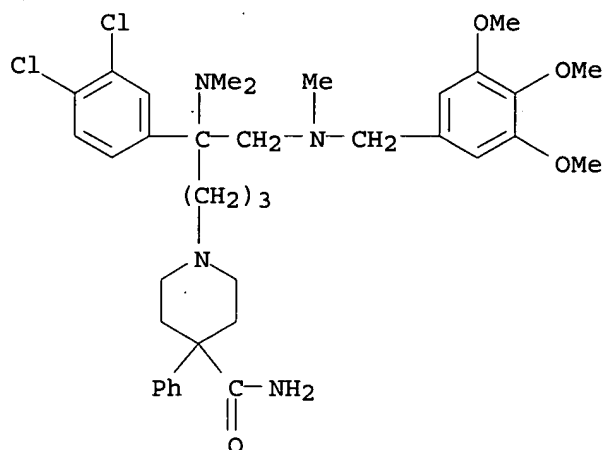


● HCl

RN 841255-95-6 CAPLUS

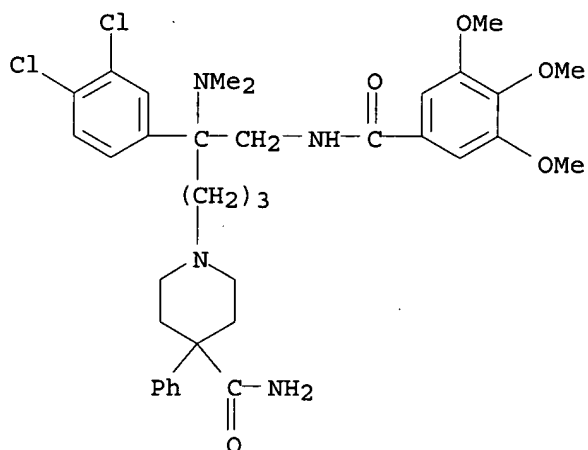
CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-(dimethylamino)-5-[methyl[(3,4,5-trimethoxyphenyl)methyl]amino]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)

10/566,252



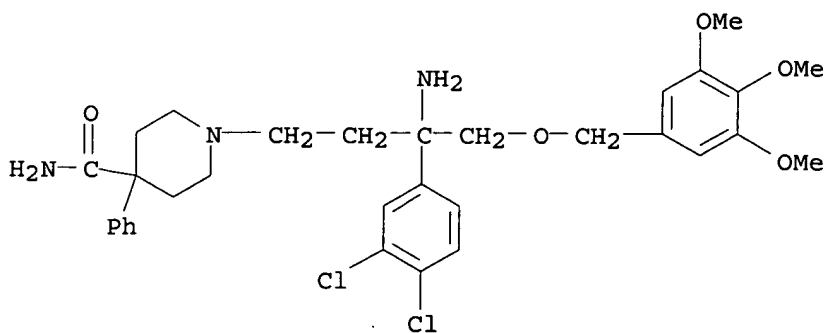
RN 841255-96-7 CAPLUS

CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-(dimethylamino)-5-[(3,4,5-trimethoxybenzoyl)aminol]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 841255-97-8 CAPLUS

CN 4-Piperidinecarboxamide, 1-[3-amino-3-(3,4-dichlorophenyl)-4-[(3,4,5-trimethoxyphenyl)methoxy]butyl]-4-phenyl- (9CI) (CA INDEX NAME)



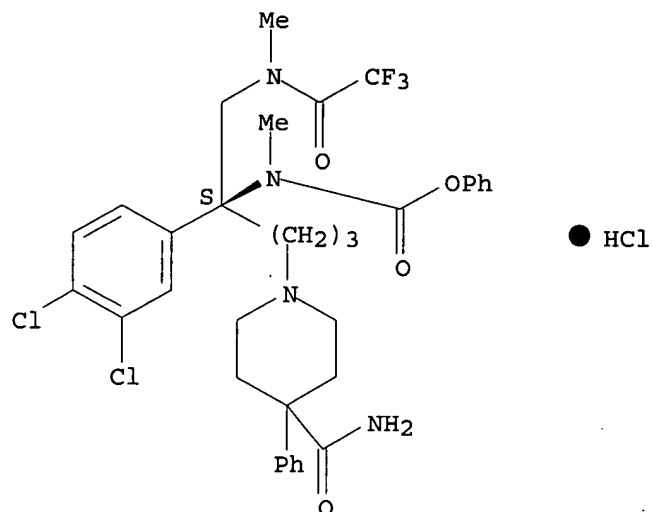
RN 841256-39-1 CAPLUS

CN Carbamic acid, [(1S)-4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-

10/566,252

dichlorophenyl)-1-[[methyl(trifluoroacetyl)amino]methyl]butyl]methyl-,  
phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 841257-84-9P

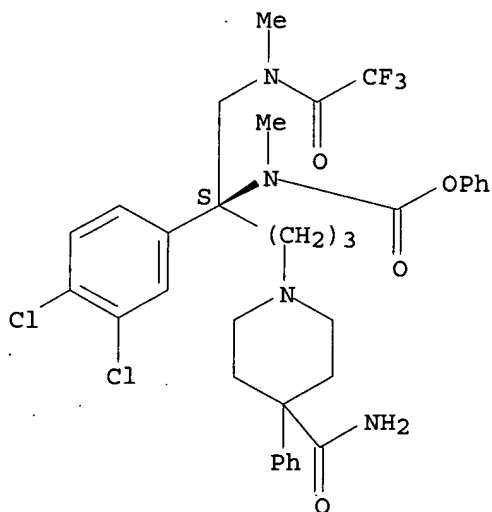
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(intermediate; preparation of (piperidylalkyl)benzylamine derivs. as  
tachykinin receptors antagonists)

RN 841257-84-9 CAPLUS

CN Carbamic acid, [(1S)-4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-  
dichlorophenyl)-1-[[methyl(trifluoroacetyl)amino]methyl]butyl]methyl-,  
phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

36

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d re 1-36

10/566,252

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN  
RE

- (1) Astra Zeneca Ab; WO 0002859 A1 2002 CAPLUS
- (2) Astra Zeneca Ab; EP 1097137 A1 2002 CAPLUS
- (3) Astra Zeneca Ab; CN 1309638 A 2002
- (4) Astra Zeneca Ab; CN 1322134 A 2002
- (5) Astra Zeneca Ab; MX 2001000268 A 2002
- (6) Astra Zeneca Ab; ZA 200100032 A 2002
- (7) Astra Zeneca Ab; NO 200100151 A 2002
- (8) Astra Zeneca Ab; MX 2001003560 A 2002
- (9) Astra Zeneca Ab; ZA 200102651 A 2002
- (10) Astra Zeneca Ab; ZA 200102658 A 2002
- (11) Astra Zeneca Ab; KR 2001083100 A 2002
- (12) Astra Zeneca Ab; JP 2002520316 A 2002
- (13) Astra Zeneca Ab; US 6365602 B1 2002 CAPLUS
- (14) Astra Zeneca Ab; BR 9912013 A 2002 CAPLUS
- (15) Astra Zeneca Ab; BR 9914333 A 2002 CAPLUS
- (16) Astra Zeneca Ab; AU 9946378 A 2002 CAPLUS
- (17) Merck & Co Inc; JP 08-505880 A 1996
- (18) Merck & Co Inc; JP 08-511522 A 1996
- (19) Merck & Co Inc; US 5869496 A 1996 CAPLUS
- (20) Merck & Co Inc; US 6013652 A 1996 CAPLUS
- (21) Merck & Co Inc; EP 681571 A1 1996 CAPLUS
- (22) Merck & Co Inc; EP 702681 A1 1996 CAPLUS
- (23) Merck & Co Inc; ZA 9403946 A 1996 CAPLUS
- (24) Merck & Co Inc; WO 9417045 A1 1996 CAPLUS
- (25) Merck & Co Inc; WO 9429309 A1 1996 CAPLUS
- (26) Merck & Co Inc; AU 9461268 A 1996 CAPLUS
- (27) Merck & Co Inc; AU 9472011 A 1996 CAPLUS
- (28) Schering Corp; US 5789422 A 1998 CAPLUS
- (29) Schering Corp; KR 2000052856 A 2001 CAPLUS
- (30) Schering Corp; JP 2001507673 A 2001
- (31) Schering Corp; NZ 334966 A 2001 CAPLUS
- (32) Schering Corp; EP 934271 A1 2001 CAPLUS
- (33) Schering Corp; AU 9674607 A 2001 CAPLUS
- (34) Schering Corp; WO 9818761 A1 2001 CAPLUS
- (35) Schering Corp; HU 9903653 A 2001
- (36) Schering Corp; MX 9903894 A 2001

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FILE 'REGISTRY' ENTERED AT 11:24:28 ON 29 SEP 2006

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L3 12 S L1 FULL

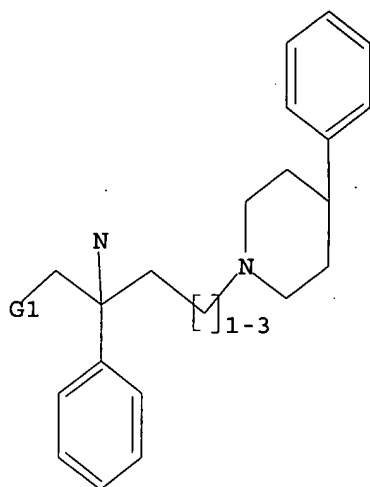
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L4 1 S L3

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L1 HAS NO ANSWERS

L1 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> => d ibib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN  
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004261534	A1	20050210	AU 2004-261534	20040802
CA 2534460	AA	20050210	CA 2004-2534460	20040802
EP 1650189	A1	20060426	EP 2004-748198	20040802
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
CN 1829689	A	20060906	CN 2004-80021890	20040802

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US 2006194841	A1	20060831	US 2006-566252	20060130
PRIORITY APPLN. INFO.:			JP 2003-205114	A 20030731
			WO 2004-JP11065	W 20040802
OTHER SOURCE(S):	MARPAT 142:219153			
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AB The title compds. I [wherein X1 = NMe, NH, or O; X2 = a single bond, NH, CONH, O, S, etc.; X3 and X4 = independently H or halo; R1 = H, alkyl, (un)substituted Ph, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = alkanoylamino, aminoalkanoyl, aminoalkanoylamino, etc.; R4 = H or forming a ring with R3; R5 = H or alkyl; m = 1 or 2; n = 0 or 1] or salts thereof are prepared as tachykinin receptors (NK) antagonists. For example, the compound II was prepared in a multi-step synthesis. II showed antagonistic activity with IC50 of 0.9 nM against human NK1. I are useful for the treatment of irritable bowel syndrome, pain, anxiety, obstructive bronchial diseases, headache, and vomiting (no data).

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(FILE 'HOME' ENTERED AT 11:23:50 ON 29 SEP 2006)

FILE 'REGISTRY' ENTERED AT 11:24:28 ON 29 SEP 2006

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 12 S L1 FULL

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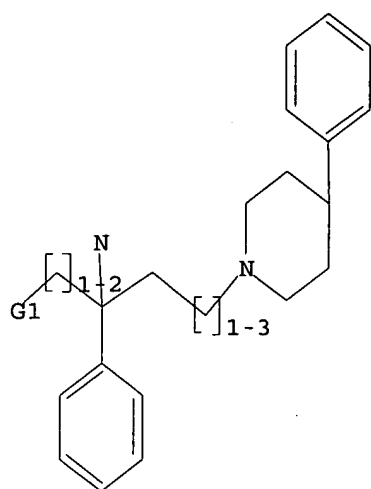
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L5 HAS NO ANSWERS

L5 STR



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G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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